Bose-Einstein condensation of self-trapping Fröhlich bipolaron in lead methylammonium halide perovskite materials

Shuang Han,[1,2] Ran An,[1,2] Wei Zhang,[1,2] Yong Sun,[1,2,*] Xin-Jun Ma,[1,2,†] Xiu-Juan Miao,[1,2] Xianglian,[1,2] Pei-Fang Li,[1,2] Tian-Ji Ou,[1,2] Quan Zhuang,[3,4] Cui-Lan Zhao,[1,2] Zhao-Hua Ding,[1,2] and Jing-Lin Xiao[1,2]

[1]*Institute of Condensed Matter Physics, Inner Mongolia Minzu University, Tongliao 028043, China*
[2]*College of Physics and Electronic Information, Inner Mongolia Minzu University, Tongliao 028043, China*
[3]*Inner Mongolia Key Laboratory of Carbon Nanomaterials, Nano Innovation Institute (NII)*
[4]*College of Chemistry and Materials Science, Inner Mongolia Minzu University, Tongliao 028000, People's Republic of China*

Bosons can gather in large quantities under certain environmental conditions to produce macroscopic quantum phenomena, forming a new state of matter known as Bose-Einstein condensation. Some quasiparticles that exist in the quantum system also produce this physical phenomenon. Notably, the bipolaron is a composite quasi-particle comprised of two polarons, and the stability and related effects of the bipolaron state have long been the focus of research in various systems. This research uses Lee-Low-Pines unitary transformation, linear combination operator, and quantum statistical theory to explore the stability and temperature effect of strong coupling Fröhlich bipolarons in methylammonium lead halide perovskite materials. It is found that the stability of bipolarons is related to self-trapping energy and effective potential. The numerical results show that the vibration frequency of bipolarons can be changed by adjusting the confined strength of parabolic potential, which leads to the change of self-trapping energy. Furthermore, the internal relative motion coordinates of bipolarons influence effective potential energy. Finally, the relationship between related physical quantities and temperature is analyzed, and it is concluded that bipolarons are stable at absolute zero, and a large number of them gather, and Bose-Einstein condensation occurs, forming Bose-Einstein condensate. This research offers some insights for exploring the properties and effects of bipolarons in perovskite materials and a theoretical idea for a Bose-Einstein condensate of boson particles.

Keywords: Bipolaron; Perovskite; Self-trapping energy; Effective potential; Temperature

I. INTRODUCTION

In condensed matter physics, Bose-Einstein condensed matter (BEC)[1–3] is a new state of matter (also called the fifth state of matter) that forms at low temperatures and high density in condensed matter. In this case, a large part of the quantum state of bosons is condensed into a single quantum state, called Bose condensation or Bose-Einstein condensation. Both theoretical verification and experimental phenomena[4] have undergone a long process. Researchers such as condensed matter physics have a strong interest in the types and properties of Bose quasi-particles through the continuous exploration theory[5, 6] and experiment[7]. Bose-Einstein condensation is also suitable for quasiparticles with integer spins in quantum systems, such as magnons[8], excitons[9], polaritons[10], and bipolarons, indicating that they are bosons that can form condensates under certain environmental conditions.Since then, scholars in various fields of physics have made theoretical analysis and experimental measurement research on Bose quasi-particles in the low-dimensional material equivalence subsystem.[11–17].

As a new structural material, the unexpected discovery of perovskite[18–20] has aroused great interest in material science and condensed matter physics. Its rich and varied electronic characteristics[21, 22] have revolutionized the development of new optoelectronic devices. Among them, methyl ammonium lead halide perovskite ($MAPbX_3$, MA=CH_3NH_3, X=Cl, Br, and I) has gradually become a hot-spot material because of its advantages such as direct band gap[23], wide spectral response, high absorption coefficient, high carrier mobility[24, 25] and long carrier diffusion coefficient[26]. It has attracted much attention because of its unique photoelectric characteristics[27], including strong light absorption and high photoluminescence quantum yield. Also, it has great prospects in practical applications such as solar cells, light-emitting diodes, lasers, and photocatalysts. A number of materials scholars have studied and discussed the effects[28–30] and properties[31] of Fermi or Bose quasi-particles in perovskite materials both experimentally and theoretically[32, 33]. The surrounding environment induces quasi-particles, and the induced interaction[34–37] has an inherent attraction so that it can lead to the formation of bound states. With the rapid development of scientific research such as information technology, people pay attention to compound quasi-particles composed of two quasi-particles. In this context, the bipolaron[38] is an important example, and its formation is considered a superconducting[39, 40] mechanism. A bound state is formed when the interaction of surrounding phonons influences two electrons (holes). There may be three types of particle combinations: electron pair, hole pair, and electron-hole pair[41, 42], whereas the first two are bipolarons, and

*Electronic address: sy19851009@126.com
†Electronic address: maxiaoguang80@126.com

the third is excitons (this paper does not elaborate too much). The spin value of electrons and holes is $\pm 1/2$, so the spin value of bipolarons is 0 or ± 1, indicating that the bipolaron is a composite Bose quasi-particle. However, the properties[43, 44] and types of bipolarons in different quantum systems have always been controversial for researchers. For example, based on the modified Lee Low Pines theory, Fobasso et al.[45] analytically studied the stability and coherence of magnetic bipolarons in asymmetric quantum dots under the action of the laser field, and they observed that the stability of bipolarons strongly depends on the electron-phonon coupling constant, magnetic field, laser frequency, and high laser field strength. Using the variational method of Huibrecht theory, Nguepnang et al.[46] studied the optical characteristics of bipolaron in single-layer transition metal chalcogenides under a magnetic field and its influence on band gap modulation from deriving the ground state energy of all the modified zero Landau levels of Fröhlich coupling constants. Abreu et al.[47] used the two-dimensional version of the Su-Schrieffer-Heeger model to study the stability of bipolaron in armchair graphene nanoribbons, which may be metallic or semiconductor, and the band gap of the semiconductor is inversely proportional to the width. And they found that the stability of bipolaron depends on the intensity of electron-phonon interaction.

Whether the Bose-Einstein condensation phenomenon occurs in the bipolaron in perovskite materials is rarely studied and analyzed by scholars. From the point of view of the stability and temperature effect of bipolarons in perovskite materials, this paper makes a theoretical discussion. As a composite Bose quasi-particle [48, 49], the properties and effects of bipolarons in perovskite materials are worth exploring and analyzing. In order to further understand the structural characteristics of perovskite materials and properties of bipolarons, the stability and temperature effect of Fröhlich bipolarons in lead methylammonium halide perovskite materials are studied using Lee-Low-Pines unitary transformation, linear combination operator, and quantum statistical theory. Compared with other theoretical methods such as peker variational method, this method transforms coordinate representation into particle representation, including any number of virtual phonon emission cases, and has a wider application range, which can be applied to zero-dimensional, one-dimensional, two-dimensional and three-dimensional systems, making the calculation simple and effective. We hope this theoretical method can be extended to some extent to open up a more novel approach for quantum systems, Bose quasi-particles, and Bose-Einstein condensation.

II. THEORETICAL MODEL

The motion of two electrons (holes) in methylammonium lead halide perovskite material is similar to that of Cooper pair, and the bipolaron is formed due to lattice constraints. We consider that the spin of the electrons (holes) is ignored and influenced by parabolic potential when the bipolaron shuttles in the crystal and has strong coupling interaction with longitudinal optical (LO) phonons, as shown in Fig. 1. The total Hamiltonian of Fröhlich bipolarons in the system is as follows:

$$\begin{aligned} H = \sum_{j=1,2} \left[\frac{p_j^2}{2m} + \sum_{\mathbf{q}} \begin{matrix} [V_q a_{\mathbf{q}} \exp(i\mathbf{q}\cdot\mathbf{r}_j) \\ + V_q^* a_{\mathbf{q}}^\dagger \exp(-i\mathbf{q}\cdot\mathbf{r}_j)] \end{matrix} \right] \\ + \frac{e^2}{\varepsilon_\infty |\mathbf{r}_1 - \mathbf{r}_2|} + \sum_{\mathbf{q}} \hbar\omega_{LO} a_{\mathbf{q}}^\dagger a_{\mathbf{q}} + \frac{1}{2} m\omega^2 r^2, \end{aligned} \tag{1}$$

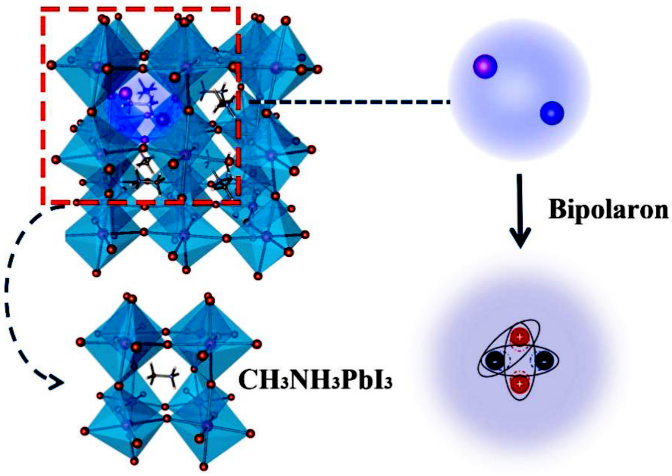

Fig. 1: Structural schematic diagram of the Fröhlich bipolarons in perovskite materials.

where first term is the kinetic energy term of electron (hole) and the interaction term between electron (hole) and phonon, while $\mathbf{r}_j$ and $\mathbf{p}_j$ are electron (hole) coordinates and momentum operators, respectively; m is that effective mass of electrons (hole); $\frac{e^2}{\varepsilon_\infty|\mathbf{r}_1-\mathbf{r}_2|}$ is the Coulomb potential between two electrons (holes); The third term is the bulk longitudinal optical phonon energy, $a_{\mathbf{q}}$ and $a_{\mathbf{q}}^\dagger$ refer to annihilation and creation operator of bulk LO phonons with wave vectors $\mathbf{q}$ and lattice vibration frequency ω_{LO}, respectively; The last term is parabolic limited potential, ω is confined strength of parabolic potential of the system in different directions. The interaction coefficient V_q in equation (1) is as follows:

$$V_q = i\left(\frac{\hbar\omega_{LO}}{q}\right)\left(\frac{\hbar}{2m\omega_{LO}}\right)^{1/4}\left(\frac{4\pi\alpha}{V}\right)^{1/2}, \tag{2}$$

where V is the volume of the crystal; α is a dimensionless strength of electron (hole)-phonon coupling.

$$\alpha = \left(\frac{e^2}{2\hbar\omega_{LO}}\right)\left(\frac{2m\omega_{LO}}{\hbar}\right)^{1/2}\left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0}\right). \tag{3}$$

where $\varepsilon_\infty\,(\varepsilon_0)$ is the optical (static) dielectric constant of the material. Since the bipolaron is a composite particle, in order to discuss the overall properties of the bipolaron, we turn the two-body problem into a monomer problem, we introduced centroid coordinates $\mathbf{R}=\frac{(\mathbf{r}_1+\mathbf{r}_2)}{2}$ and relative coordinates $\mathbf{r}=\mathbf{r}_1-\mathbf{r}_2$ for the electron (hole) pair, allowing us to rewrite the Hamiltonian of the Fröhlich bipolarons in the system as follows:

$$\begin{aligned} H &= \frac{\mathbf{P}^2}{2M}+\frac{\mathbf{p}^2}{2\mu}+\frac{\beta}{r}+\sum_{\mathbf{q}}\hbar\omega_{LO}a_{\mathbf{q}}^{\dagger}a_{\mathbf{q}} \\ &+\frac{1}{2}M\omega^2R^2+\frac{1}{2}\mu\omega^2r^2 \\ &+2\sum_{\mathbf{q}}\cos\frac{\mathbf{q}\cdot\mathbf{r}}{2}\left[\begin{array}{l} V_q a_{\mathbf{q}}\exp\left(i\mathbf{q}\cdot\mathbf{R}\right) \\ +V_q^* a_{\mathbf{q}}^{\dagger}\exp\left(-i\mathbf{q}\cdot\mathbf{R}\right)\end{array}\right], \end{aligned} \tag{4}$$

where $\mathbf{P}$ and $\mathbf{p}$ are centroid momentum and relative momentum, respectively. M and μ refer to centroid mass and reduced mass, respectively; $\beta{=}e^2/\varepsilon_\infty$ is the Coulomb potential strength between two electrons (holes); r is internal relative motion coordinates of bipolarons. This paper attempts to quantize the related quantity of centroid motion. We introduced production $B^\dagger$ and annihilation B operators for centroid momentum $\mathbf{P}$ and centroid coordinates $\mathbf{R}$ in the following equation[50]:

$$\begin{aligned} \mathbf{P}_j &= \left(\frac{M\hbar\lambda}{2}\right)^{1/2}\left(B_j+B_j^{\dagger}\right), \\ \mathbf{R}_j &= i\left(\frac{\hbar}{2M\lambda}\right)^{1/2}\left(B_j-B_j^{\dagger}\right). \end{aligned} \tag{5}$$

where λ is a variational parameter. Substituting Eq. (5) into (4) and performing Lee-Low-Pines unitary transformation[51]

$$U=\exp\sum_{\mathbf{q}}\left(a_{\mathbf{q}}^{\dagger}f_q-a_{\mathbf{q}}f_q^*\right). \tag{6}$$

where $f_q\left(f_q^*\right)$ is a variational parameter, then Eq. (4) can be rewritten as:

$$\begin{aligned} H &= \frac{\mathbf{p}^2}{2\mu}+\frac{\hbar\lambda}{2}\left(\sum_j B_j^{\dagger}B_j+1\right)+\frac{\hbar\lambda}{4}\sum_j\left(B_j^{\dagger}B_j^{\dagger}+B_jB_j\right)+\frac{1}{2}\mu\omega^2r^2+\frac{\beta}{r} \\ &-\frac{\hbar\omega^2}{4\lambda}\sum_{j=1}^{2}\left(B_j^{\dagger}B_j^{\dagger}+B_jB_j\right)+\frac{\hbar\omega^2}{4\lambda}\left(\sum_{j=1}^{2}2B_j^{\dagger}B_j+2\right)+\sum_q\hbar\omega_{LO}\left(a_q^{\dagger}+f_q^*\right)\left(a_q+f_q\right) \\ &+2\sum_q\cos\frac{q\cdot r}{2}\left[V_q\left(a_q+f_q\right)\exp\left(-\frac{\hbar q^2}{4M\lambda}\right)\exp\left[-\left(\frac{\hbar}{2M\lambda}\right)^{1/2}\sum_j q_jB_j^{\dagger}\right]\exp\left[\left(\frac{\hbar}{2M\lambda}\right)^{1/2}\sum_j q_jB_j\right]+h.c\right] \\ &+\frac{\hbar^2}{\mu}\sum_{q,q'}\nabla_r f_q\cdot\nabla_r f_{q'}^*a_q^{\dagger}a_q+\frac{\hbar^2}{2\mu}\sum_q\left|\nabla_r f_q\right|^2-\frac{\hbar^2}{2\mu}\sum_{q,q'}\left(\nabla_r f_q\cdot\nabla_r f_{q'}a_q^{\dagger}a_{q'}^{\dagger}+\nabla_r f_q^*\cdot\nabla_r f_{q'}^*a_qa_{q'}\right) \\ &-\frac{\hbar^2}{\mu}\sum_q\left(a_q^{\dagger}\nabla_r f_q-a_q\nabla_r f_q^*\right)\cdot\nabla_r-\frac{\hbar^2}{2\mu}\sum_q\left(a_q^{\dagger}\nabla_r^2 f_q-a_q\nabla_r^2 f_q^*\right) \end{aligned} \tag{7}$$

The ground state wave function of the system is selected as

$$|\psi\rangle=|\varphi\left(r\right)\rangle\,|0\rangle_a|0\rangle_B, \tag{8}$$

where $|\varphi\left(r\right)\rangle$ is a wave function of relative motion of bipolaron. This model only analyzes the motion of the center of mass of bipolaron, and only the second quantization is carried out, and the normalized wave function is taken, then $\langle\varphi\left(r\right)\mid\varphi\left(r\right)\rangle=1.$; $|0\rangle_a$ is the unperturbed zero phonon state and $|0\rangle_B$ represents the vacuum state of the operator b , which satisfies the following relation:

$$a_{\mathbf{q}}|0\rangle_a=B_j|0\rangle_B=0. \tag{9}$$

The details of the calculation are presented in the Appendix. The expression of vibration frequency is obtained by the variation of λ with Eq. (18):

$$\lambda^2-\frac{4\alpha}{3}\sqrt{\frac{2\omega_{LO}}{\pi}}\lambda^{3/2}+2\alpha\sqrt{\frac{2}{\pi\omega_{LO}}}\lambda^{5/2}-\frac{2\omega^2}{3}=0, \tag{10}$$

Then $F(\lambda)$ can be understood as the effective Hamiltonian H_{eff}, as follows:

$$H_{eff} = \frac{\mathbf{p}^2}{2\mu} - E_{tr} + V_{eff}, \tag{11}$$

$$\begin{aligned} E_{tr} = & -\frac{3}{4}\hbar\lambda_0 + \frac{2\sqrt{2}}{\sqrt{\pi}}\alpha\hbar\omega_{LO}\left(\frac{\lambda_0}{\omega_{LO}}\right)^{1/2} \\ & -\frac{\sqrt{2}}{\sqrt{\pi}}\alpha\hbar\omega_{LO}\left(\frac{\lambda_0}{\omega_{LO}}\right)^{3/2} - \frac{\hbar\omega^2}{2\lambda_0}, \end{aligned} \tag{12}$$

$$\begin{aligned} V_{eff} &= V_{Coul} + V_{conf} + V_{e-LO}, \\ V_{Coul} &= \frac{\beta}{r}, \\ V_{conf} &= \frac{1}{4}\mu\omega^2 r^2, \\ V_{e-LO} &= -\frac{2}{\sqrt{\pi}}\alpha\hbar\omega_{LO}\left(\frac{\lambda_0}{\omega_{LO}}\right)^{3/2} \\ & \exp\left(-\frac{M\lambda_0}{\hbar}r^2\right) \\ & - 2\alpha\hbar\sqrt{\frac{\hbar\omega_{LO}}{M}}\frac{1}{r}, \end{aligned} \tag{13}$$

where E_{tr} is the self-trapping energy of bipolaron; V_{eff} is the effective potential of bipolaron which refers to a potential energy that combines multiple potential energies with the same or opposite effects; V_{Coul} is Coulomb potential; V_{conf} is a parabolic potential of the system; V_{e-LO} arises by electron-LO phonon interaction, that is, induced potential. LO-phonon mean number is expressed as follows:

$$\begin{aligned} N = & 2\alpha\sqrt{\frac{\lambda_0}{\pi\omega_{LO}}} + \frac{2\alpha}{r}\sqrt{\frac{\hbar}{m\omega_{LO}}} \\ & \left(1 - erfc\left(\sqrt{\frac{M\lambda_0}{2\hbar}}r\right)\right). \end{aligned} \tag{14}$$

III. TEMPERATURE EFFECT

The lattice vibration caused by lattice distortion not only excites phonons, but also reacts to bound states when perovskite materials are placed at a limited temperature. Its statistical average of various states is used to describe the properties of bipolaron. Based on the quantum statistical theory[52], the statistical mean number of the bulk LO phonons is determined as follows:

$$\overline{N} = \left[\exp\left(\frac{\hbar\omega_{LO}}{K_B T}\right) - 1\right]^{-1} \tag{15}$$

where K_B is Boltzmann's constant and T is temperature. The self-consistent calculation is used between Eqs. (14) and (15), and the relationship between vibration frequency and temperature is obtained. Similarly, the bipolaron self-trapping energy and effective potential depend on the temperature in Eqs. (11), (12) and (13).

IV. RESULTS AND DISCUSSION

Based on numerical calculations, it is found that vibration frequency and self-trapping energy of a strongly coupled Fröhlich bipolarons are related to the confined strength of parabolic potential, whereas effective potential and LO-phonon mean number are related to internal relative motion coordinates of bipolarons. The relationship between temperature and vibration frequency, an average number of LO phonons, self-trapping energy, and effective potential are all explored. Strong coupling electron (hole)-phonon interaction is considered to verify the stability and temperature effect of Fröhlich bipolarons, and model parameters of lead methylammonium halide perovskite material (Table 1) are used for numerical calculation and discussion.

TABLE I: Physical parameter values used in the numerical calculation[53, 54] (where $m_0 = 9.1 \times 10^{-31} kg$)

Parameter	$MAPbI_3$	$MAPbBr_3$	$MAPbCl_3$
Phonon energy $\hbar\omega_{LO}(meV)$	11.5	15.3	26.4
Coupling constant α	1.72	1.69	2.17
Effective mass $M(kg)$	$0.104m_0$	$0.117m_0$	$0.2m_0$

As a fundamental physical quantity describing characteristics of carriers, the vibration frequency is strongly influenced by the confined strength of parabolic potential. Fig. 2 depicts that the relationship between (a) the vibration frequency and (b) self-trapping energy of bipolaron in three kinds of methylamine lead halide perovskite materials with different halogen elements and the confined strength of parabolic potential. The bipolaron is influenced by parabolic potential. With the increase of confined strength, the motion of bipolaron is restricted to some extent, which leads to the increase of vibration frequency, showing a unique quantum size effect, which is beneficial to the stability of bipolaron. This is due to the influence of lattice squeezing and distortion, two polarons are coupled into bound Bose quasi-particles and move freely together. When the bipolaron is in a relatively stable state and interacts with the surrounding phonons, the lattice vibrates. If this coupling is weak, the bipolaron may be scattered by phonons; However, when it is very strong, it leads to self-trapping of bipolarons, resulting in self-trapping energy. The bipolaron is influenced by conditions similar to phonons, which leads to the change of potential field and the generation of potential barrier. When the barrier reacts on the bipolaron, it is trapped in this barrier to form a self-trapping bipolaron. It can be clearly seen from equations (10) and (11) that

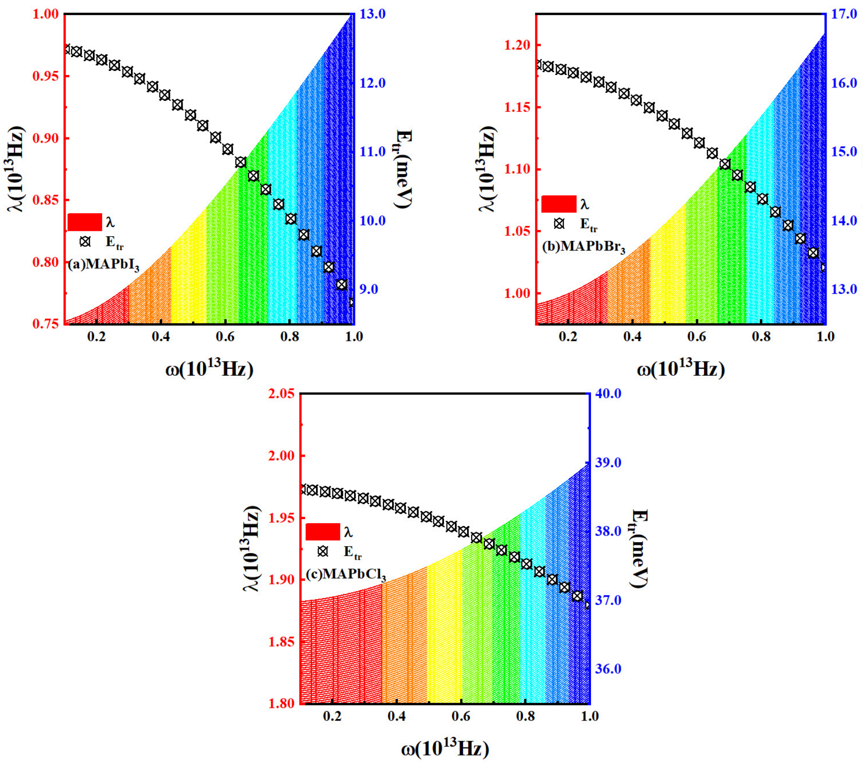

Fig. 2: The vibration frequency and self-trapping energy are linearly correlated with confined strength of parabolic potential. (a)$MAPbI_3$. (b)$MAPbBr_3$. (c)$MAPbCl_3$.

the confined strength of parabolic potential changes the magnitude of vibration frequency, thus changing the self-trapping energy. As shown in Fig. 2, with the increase of confined strength, bipolaron increases and self-trapping energy decreases. This is because self-trapping leads to the influence of bipolaron on lattice distortion, forming a relatively compact phonon cloud, strongly inhibiting the energy of bipolaron passing through perovskite material, limiting the motion of bipolaron, reducing the motion speed, promoting the stability of self-trapping bound state, and a large number of bipolarons gather to form Bose-Einstein condensate. Lühmann et al.[55] theoretically studied enhanced localization of bosons by fermion atoms in three-dimensional optical lattices and found a self-trapping of bosons for attractive boson-fermion interaction. Due to this mutual interaction, the fermion orbitals are substantially squeezed, which leads to a strong deformation of the effective potential for bosons. Similarly, our theory proves that phonon coupling promotes lattice vibration, results in self-trapping of bipolarons, generates self-trapping energy and is influenced by the confined strength of parabolic potential. In fact, the energy of bipolaron is less than double that of polaron, which is due to the Coulomb interaction between bipolarons. By calculating the self-trapping energy of bipolaron, it can be confirmed that bipolaron is a possible Bose quasi-particle in the system. Casteels et al.[56] extended the variational Feynman form of polaron to the full coupling treatment of bipolaron, and applied it to two impurity atoms in Bose-Einstein condensate, indicating that if the coupling strength of polaron is large enough, the impurity will form a bound state (bipolaron).

The influence factors of Bose-Einstein condensate are also related to the interaction between electrons (holes) and phonons, which also plays an important role in solving the effective potential problem composed of multiple particles with the same or opposite effects. Fig. 3 shows the relationship between the relative motion coordinates inside the bipolaron of (a) effective potential and (b) LO-phonon mean number. In a given interval , the smaller the relative motion coordinates in the bipolaron, the greater the absolute value of effective potential energy and the more LO-phonon mean number. That is to say, when the distance between two polarons is closer, the effective interaction between electrons (holes) and phonons is stronger, and the effective potential energy is increased, which can stimulate the interaction between electrons (holes) and more

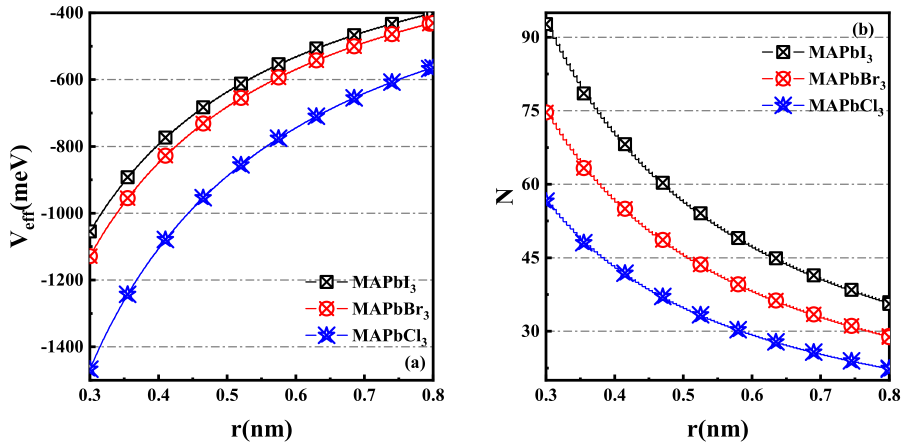

Fig. 3: The (a) effective potential and (b) LO-phonon mean number are linearly correlated with internal relative motion coordinates of bipolaron.

phonons, produce a larger LO-phonon mean number, gather a large number of Bose quasi-particles, limit the motion of bipolars, promote more stable bound states, and form Bose-Einstein condensate. As the interaction between two electrons (holes) caused by the coupling of electrons (holes) and phonons is mutually attractive in the lead halide perovskite material of methylammonium, the value of effective potential is always less than zero. Kashirina et al.[57] performed theoretical investigation on the structure of one-dimensional bipolaron, taking into account three types of correlation effects, such as interelectronic correlations caused by the direct dependence of the wave function on the distance between electrons and the one-center and two-center correlations. Gaussian orbitals with exponentially-correlated multipliers were used for variational calculations. Unlike in a three-dimensional system, it is shown that in the domain of one-dimensional optical bipolaron, two-center bipolaron is formed. Drescher et al.[58] have investigated the problem of a force between particles induced by an interacting Bose-Einstein condensed medium by minimizing local and non-local Gross Pitaevskii energy functionals. Experimentally, induced interactions are expected to lead to an energy shift depending on impurity concentration, which may be probed by radio-frequency spectroscopy [59, 60].To investigate the distance dependence, the impurities can be confined to individual microtraps. This is related to the analysis of our model.

Finally, the temperature effect of Bose-Einstein condensation is discussed. Fig. 4 describes the relationship between (a) vibration frequency, (b) LO-phonon mean number, (c) self-trapping energy, (d) effective potential and temperature. It is not difficult to find that when the temperature is close to absolute zero, the physical quantity of bipolarons remains stable, and a large number of gathered bipolarons have similar vibration frequency, self-trapping energy and effective potential energy. It shows that the bound state formed by bipolaron and Bose-Einstein condensate are relatively stable. When the temperature is heated continuously, the related physical quantities change continuously and the equilibrium state is broken. The LO-phonon mean number is larger at lower temperature, which leads to higher vibration frequency, lower self-trapping energy, higher absolute value of effective potential, more stable bound state of bipolaron, and more possibility of forming Bose-Einstein condensate. This is because the higher the temperature of methylammonium lead halide perovskite material system, the more intense the movement between electrons (holes) and phonons, which inhibits the coupling interaction between bipolarons and more phonons and the self-trapping effect of bipolarons. On the contrary, when the temperature is close to absolute zero, bipolaron states can combine and form a condensate, thus Bose-Einstein condensation occurs. Camacho et al. [61] proved that two polarons can combine to form bound bipolaron states. Its emergence is caused by induced non-local interaction mediated by density oscillations in condensate, and an effective Schrödinger equation describing arbitrary strong impurity-boson interaction is derived by field theory. Furthermore, they compared with quantum Monte Carlo simulations and found remarkable consistency, emphasizing the predictive ability of developed theory. It is found that the formation of bipolaron usually requires strong impurity interaction, which exceeds the effectiveness of the more commonly used weak coupling method that leads to local Yukawa-type interaction.

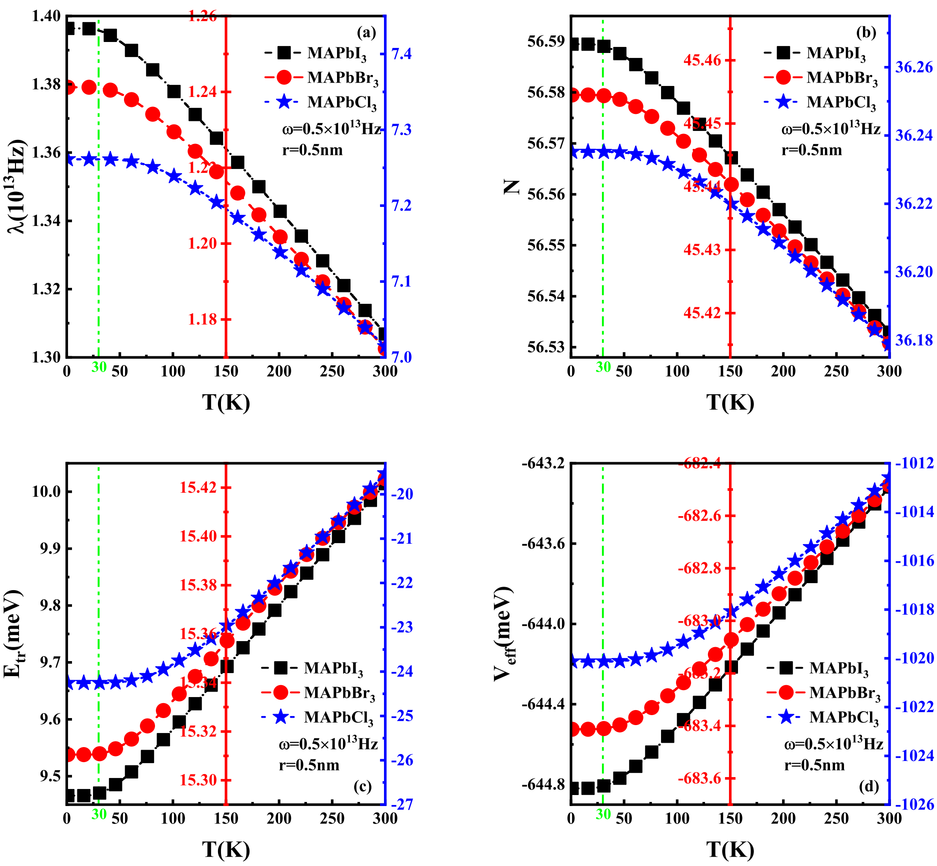

Fig. 4: The (a) vibration frequency, (b) LO-phonon mean number, (c) self-trapping energy, and (d) effective potential energy are linearly correlated with temperature.

V. CONCLUSION

The present research examines the stability and temperature impact of bipolaron in perovskite materials. This study utilizes linear combination operator, unitary transformation, and quantum statistical theory to analyze the changes in vibration frequency, self-trapping energy, and effective potential of bipolaron in lead methylammonium halide perovskite materials. Furthermore, the above three physical parameters and LO-phonon mean number with temperature under strong electron-LO phonon coupling conditions are analyzed. It is not difficult to know that the influencing factors of Bose-Einstein condensation include temperature, interaction, velocity and quantity of quasi-particles, etc. We analyze some physical quantities of bipolaron and explore the fundamental reason for changing its value. Numerical results showed that tuning the finite strength of parabolic potential affects the vibrational frequency of bipolaron, which in turn affects self-trapping energy, thereby suppressing the stability of bipolaron. Furthermore, the internal relative motion coordinates of bipolaron affect effective potential and LO-phonon mean number. The smaller the internal relative motion coordinates, are more stable the bound state of bipolaron. Finally, the results showed that bipolaron vibrational frequency, self-trapping energy, effective potential, and LO-phonon mean number are relatively stable when the temperature reaches near zero, providing a new theoretical idea for forming bipolaron Bose-Einstein condensates. In this study, the self-trapping energy and effective potential are calculated, and the temperature effect shows that the bipolaron is a Bose quasi-particle in perovskite materials and is related to Bose-Einstein condensate, providing some insights for exploring and understanding the properties and effects of bipolarons and Bose-Einstein condensation, and lays a foundation for further exploring superfluid superconductivity.

VI. APPENDIX

We obtain

$$
\begin{aligned}
F(\lambda) &= \langle \psi \left| U^{-1} H U \right| \psi \rangle \\
&= \langle \varphi(r) | F(\lambda) | \varphi(r) \rangle \\
H_{eff} &= \min F(\lambda)
\end{aligned}
\tag{16}
$$

where H_{eff} is called the effective Hamiltonian, and we get

$$
\begin{aligned}
F(\lambda) = &\frac{3}{4}\hbar\lambda + \frac{p^2}{2\mu} + \frac{1}{2}\mu\omega^2 r^2 + \frac{\beta}{r} + \frac{\hbar\omega^2}{2\lambda} \\
&+ \sum_q \hbar\omega_{LO} |f_q|^2 + \frac{\hbar^2}{2\mu}\sum_q |\nabla_r f_q|^2 + 2\sum_q \cos\frac{q\cdot r}{2}\left[V_q f_q \exp\left(-\frac{\hbar q^2}{4M\lambda}\right) + h.c\right]
\end{aligned}
\tag{17}
$$

Through the variation of Eq.17, f_q is obtained. f_q by inserting $F(\lambda)$ and replacing summation with integral, we get

$$
\begin{aligned}
F(\lambda) = &-\frac{\hbar^2}{2\mu}\nabla_r^2 + \frac{1}{2}\mu\omega^2 r^2 + \frac{\beta}{r} + \frac{3}{4}\hbar\lambda + \frac{\hbar\omega^2}{2\lambda} \\
&+ \frac{\sqrt{2}}{\sqrt{\pi}}\alpha\hbar\omega_{LO}\left(\frac{\lambda}{\omega_{LO}}\right)^{\frac{3}{2}}\left(1 - \exp\left(-\frac{m\lambda}{\hbar}r^2\right)\right) \\
&- \frac{2\sqrt{2}}{\sqrt{\pi}}\alpha\hbar\omega_{LO}\left(\frac{\lambda}{\omega_{LO}}\right)^{\frac{1}{2}} - \sqrt{2}\alpha\hbar\sqrt{\frac{\hbar\omega_{LO}}{m}}\frac{1}{r}
\end{aligned}
\tag{18}
$$

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